



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:30 AM UTC

PDB ID : 1TNF / pdb_00001tnf
Title : THE STRUCTURE OF TUMOR NECROSIS FACTOR-ALPHA AT 2.6
ANGSTROMS RESOLUTION. IMPLICATIONS FOR RECEPTOR BIND-
ING
Authors : Eck, M.J.; Sprang, S.R.
Deposited on : 1989-08-25
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

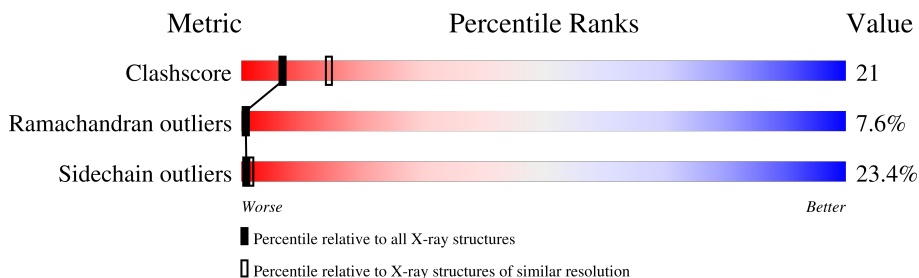
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	157	31% 41% 17% 8% .
1	B	157	29% 44% 18% 6% .
1	C	157	27% 45% 17% 8% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3552 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TUMOR NECROSIS FACTOR-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1184	757	204	221	2			
1	B	152	Total	C	N	O	S	0	0	0
			1184	757	204	221	2			
1	C	152	Total	C	N	O	S	0	0	0
			1184	757	204	221	2			

There are 3 discrepancies between the modelled and reference sequences:

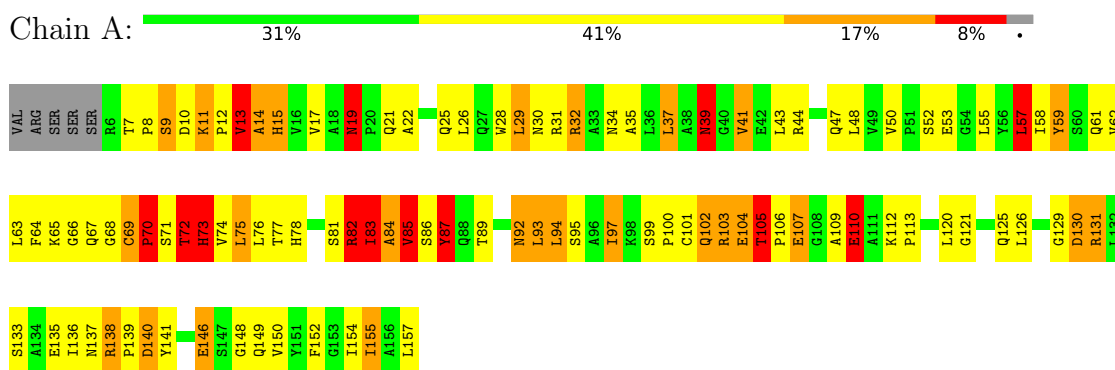
Chain	Residue	Modelled	Actual	Comment	Reference
A	45	ASP	LEU	conflict	UNP P01375
B	45	ASP	LEU	conflict	UNP P01375
C	45	ASP	LEU	conflict	UNP P01375

3 Residue-property plots

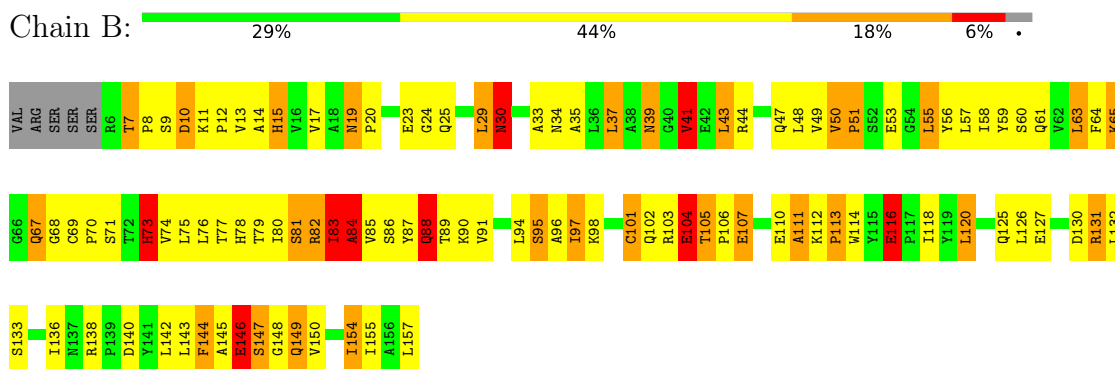
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

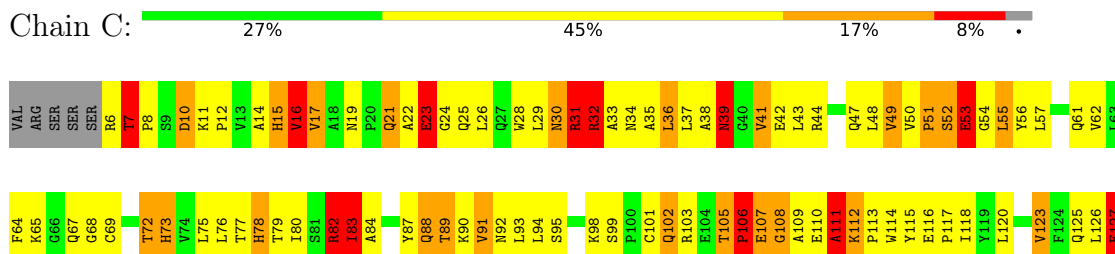
• Molecule 1: TUMOR NECROSIS FACTOR-ALPHA



• Molecule 1: TUMOR NECROSIS FACTOR-ALPHA



• Molecule 1: TUMOR NECROSIS FACTOR-ALPHA





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.00Å 95.00Å 117.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.230 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3552	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.22	6/1211 (0.5%)	2.35	72/1649 (4.4%)
1	B	1.27	5/1211 (0.4%)	2.28	69/1649 (4.2%)
1	C	1.24	7/1211 (0.6%)	2.30	67/1649 (4.1%)
All	All	1.24	18/3633 (0.5%)	2.31	208/4947 (4.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	3
All	All	0	7

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	VAL	CA-CB	8.46	1.65	1.54
1	B	83	ILE	CA-CB	8.39	1.63	1.53
1	A	72	THR	CA-CB	7.35	1.65	1.53
1	A	78	HIS	CD2-NE2	-7.30	1.29	1.37
1	A	15	HIS	CD2-NE2	-7.16	1.29	1.37
1	B	15	HIS	CD2-NE2	-7.08	1.30	1.37
1	C	15	HIS	CD2-NE2	-7.04	1.30	1.37
1	C	78	HIS	CD2-NE2	-6.75	1.30	1.37
1	C	41	VAL	CA-CB	6.74	1.61	1.54
1	C	73	HIS	CD2-NE2	-6.56	1.30	1.37
1	A	87	TYR	CA-CB	6.51	1.61	1.52
1	B	78	HIS	CD2-NE2	-6.25	1.30	1.37
1	B	73	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	73	HIS	CD2-NE2	-6.20	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	HIS	CG-ND1	-6.05	1.31	1.38
1	C	15	HIS	CG-ND1	-5.78	1.31	1.38
1	C	77	THR	CA-CB	5.72	1.63	1.53
1	A	83	ILE	CA-CB	5.55	1.60	1.53

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	GLU	N-CA-C	13.97	131.97	109.76
1	A	73	HIS	CA-CB-CG	-13.83	99.97	113.80
1	A	74	VAL	N-CA-C	12.12	121.77	110.74
1	C	113	PRO	N-CA-C	11.72	129.67	111.15
1	C	39	ASN	CA-CB-CG	10.94	123.54	112.60
1	B	88	GLN	CA-CB-CG	10.73	135.56	114.10
1	A	138	ARG	NE-CZ-NH2	10.25	128.43	119.20
1	A	140	ASP	CA-CB-CG	9.60	122.20	112.60
1	A	37	LEU	N-CA-C	-9.47	92.54	108.26
1	C	106	PRO	N-CA-C	9.35	131.73	112.47
1	C	87	TYR	N-CA-C	-9.32	92.19	108.23
1	C	15	HIS	CA-CB-CG	-9.26	104.54	113.80
1	B	88	GLN	OE1-CD-NE2	-9.05	113.55	122.60
1	B	149	GLN	CG-CD-NE2	9.03	129.94	116.40
1	B	149	GLN	OE1-CD-NE2	-8.77	113.83	122.60
1	B	10	ASP	CA-CB-CG	8.75	121.35	112.60
1	A	73	HIS	N-CA-C	8.61	124.06	107.44
1	C	38	ALA	O-C-N	8.50	132.94	123.25
1	B	39	ASN	CB-CG-ND2	8.25	128.78	116.40
1	B	149	GLN	N-CA-C	-8.12	105.37	114.62
1	A	146	GLU	CA-C-O	-8.09	110.33	120.28
1	B	111	ALA	N-CA-C	8.09	128.03	110.80
1	A	102	GLN	N-CA-C	-8.02	92.01	107.57
1	C	140	ASP	CA-CB-CG	7.96	120.56	112.60
1	C	107	GLU	CA-CB-CG	7.87	129.84	114.10
1	B	144	PHE	CA-CB-CG	7.87	121.67	113.80
1	B	50	VAL	N-CA-C	7.86	115.69	107.76
1	B	138	ARG	NE-CZ-NH2	7.82	126.24	119.20
1	B	19	ASN	CB-CG-ND2	7.79	128.09	116.40
1	C	88	GLN	CA-CB-CG	-7.74	98.62	114.10
1	C	112	LYS	CA-C-N	7.67	127.72	119.90
1	C	112	LYS	C-N-CA	7.67	127.72	119.90
1	A	84	ALA	N-CA-C	7.64	121.27	110.50
1	C	72	THR	CA-CB-OG1	-7.52	98.31	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	ASN	OD1-CG-ND2	-7.52	115.08	122.60
1	C	25	GLN	N-CA-C	7.50	126.77	110.80
1	B	140	ASP	CA-CB-CG	7.42	120.02	112.60
1	C	32	ARG	NE-CZ-NH2	7.38	125.84	119.20
1	B	10	ASP	N-CA-C	-7.33	101.42	110.65
1	B	33	ALA	N-CA-C	7.30	121.28	112.38
1	A	93	LEU	N-CA-C	7.19	122.11	113.12
1	A	130	ASP	CA-CB-CG	7.15	119.75	112.60
1	A	152	PHE	CA-CB-CG	7.10	120.90	113.80
1	A	22	ALA	CA-C-O	7.07	130.61	120.51
1	B	131	ARG	NE-CZ-NH2	7.05	125.55	119.20
1	A	148	GLY	O-C-N	7.01	131.81	122.70
1	C	73	HIS	CB-CG-CD2	-6.98	122.13	131.20
1	A	107	GLU	N-CA-C	6.94	125.59	110.80
1	A	81	SER	CA-CB-OG	6.92	124.94	111.10
1	A	87	TYR	CA-CB-CG	6.92	126.36	113.90
1	C	7	THR	CA-C-N	6.90	128.47	119.84
1	C	7	THR	C-N-CA	6.90	128.47	119.84
1	C	82	ARG	CA-C-N	-6.88	113.77	122.43
1	C	82	ARG	C-N-CA	-6.88	113.77	122.43
1	A	69	CYS	CA-CB-SG	-6.85	98.65	114.40
1	B	55	LEU	O-C-N	-6.84	115.22	123.29
1	C	7	THR	CA-C-O	-6.82	113.34	119.75
1	C	83	ILE	CA-CB-CG1	6.79	121.94	110.40
1	B	116	GLU	CA-C-O	-6.77	113.52	120.63
1	C	43	LEU	N-CA-C	-6.75	98.20	109.07
1	B	82	ARG	CA-CB-CG	6.73	127.56	114.10
1	C	102	GLN	CA-C-O	-6.73	113.74	121.47
1	C	21	GLN	N-CA-C	-6.71	104.25	113.18
1	B	97	ILE	CA-C-O	-6.69	114.27	120.22
1	C	83	ILE	CA-CB-CG2	-6.65	99.19	110.50
1	C	16	VAL	N-CA-CB	-6.65	100.53	111.44
1	B	74	VAL	CA-C-O	-6.65	114.18	121.29
1	C	53	GLU	N-CA-C	-6.64	96.65	110.80
1	A	53	GLU	N-CA-C	-6.62	99.24	109.76
1	B	7	THR	N-CA-CB	-6.58	98.66	110.37
1	B	145	ALA	N-CA-C	-6.47	102.50	111.81
1	C	89	THR	CA-CB-OG1	-6.45	99.93	109.60
1	C	23	GLU	CB-CG-CD	6.39	123.47	112.60
1	A	137	ASN	CA-C-N	-6.36	115.14	123.34
1	A	137	ASN	C-N-CA	-6.36	115.14	123.34
1	A	85	VAL	CA-CB-CG2	-6.34	99.63	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	28	TRP	CG-CD2-CE3	6.34	140.24	133.90
1	B	89	THR	N-CA-C	-6.31	100.60	109.69
1	A	83	ILE	CB-CA-C	6.29	120.25	112.45
1	C	39	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	C	49	VAL	N-CA-C	-6.28	99.38	108.36
1	B	39	ASN	N-CA-C	6.27	120.04	111.39
1	B	88	GLN	CG-CD-NE2	6.27	125.80	116.40
1	C	111	ALA	N-CA-C	6.26	124.14	110.80
1	A	41	VAL	N-CA-C	-6.25	100.64	108.89
1	C	92	ASN	CA-CB-CG	-6.25	106.35	112.60
1	C	87	TYR	CA-CB-CG	6.24	125.13	113.90
1	B	83	ILE	N-CA-C	-6.21	98.04	106.85
1	B	73	HIS	O-C-N	6.20	131.21	123.28
1	A	105	THR	CA-C-O	6.17	124.73	120.47
1	C	10	ASP	CA-C-O	6.14	128.08	121.02
1	C	44	ARG	O-C-N	-6.13	114.43	122.59
1	B	88	GLN	N-CA-CB	-6.06	100.24	110.49
1	C	149	GLN	N-CA-CB	-6.06	100.21	110.51
1	A	86	SER	N-CA-C	-6.05	104.01	112.12
1	A	13	VAL	CB-CA-C	-6.05	101.87	110.82
1	A	34	ASN	N-CA-C	-6.04	98.52	108.49
1	A	57	LEU	N-CA-C	-6.04	98.68	108.52
1	B	138	ARG	NE-CZ-NH1	-5.98	115.52	121.50
1	A	50	VAL	N-CA-C	5.97	114.80	108.95
1	B	147	SER	N-CA-C	-5.96	98.10	110.80
1	A	99	SER	N-CA-C	-5.95	100.00	109.04
1	C	127	GLU	CA-CB-CG	-5.89	102.31	114.10
1	A	104	GLU	CB-CG-CD	5.88	122.60	112.60
1	A	125	GLN	OE1-CD-NE2	-5.88	116.72	122.60
1	C	15	HIS	N-CA-C	-5.88	97.39	107.61
1	B	55	LEU	N-CA-C	-5.87	99.63	109.07
1	B	64	PHE	CA-CB-CG	5.85	119.65	113.80
1	A	44	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	B	90	LYS	CA-C-N	-5.84	115.95	123.19
1	B	90	LYS	C-N-CA	-5.84	115.95	123.19
1	C	88	GLN	CB-CG-CD	5.83	122.51	112.60
1	A	138	ARG	NE-CZ-NH1	-5.82	115.68	121.50
1	C	44	ARG	CA-C-O	-5.82	112.19	120.51
1	C	123	VAL	N-CA-CB	-5.78	104.19	111.41
1	A	53	GLU	CB-CG-CD	5.76	122.39	112.60
1	B	113	PRO	N-CA-CB	-5.75	98.58	103.36
1	B	19	ASN	OD1-CG-ND2	-5.75	116.85	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	ASN	OD1-CG-ND2	-5.70	116.90	122.60
1	A	78	HIS	CA-CB-CG	-5.69	108.11	113.80
1	B	101	CYS	O-C-N	-5.69	116.74	123.22
1	A	94	LEU	N-CA-C	-5.67	100.08	108.99
1	A	82	ARG	CA-C-N	-5.66	116.36	122.59
1	A	82	ARG	C-N-CA	-5.66	116.36	122.59
1	B	91	VAL	N-CA-CB	5.66	118.94	111.25
1	B	41	VAL	N-CA-C	-5.64	101.77	109.55
1	B	39	ASN	OD1-CG-ND2	-5.63	116.97	122.60
1	A	131	ARG	CA-CB-CG	5.62	125.33	114.10
1	A	11	LYS	N-CA-C	-5.61	101.85	110.32
1	B	87	TYR	CA-CB-CG	5.59	123.97	113.90
1	C	7	THR	O-C-N	-5.59	116.33	121.30
1	A	28	TRP	CE2-CD2-CG	-5.58	100.50	107.20
1	A	25	GLN	O-C-N	-5.58	117.38	123.52
1	B	30	ASN	N-CA-C	-5.58	101.14	109.96
1	A	133	SER	O-C-N	-5.58	116.13	123.16
1	A	82	ARG	NE-CZ-NH2	5.56	124.21	119.20
1	C	53	GLU	CB-CG-CD	5.55	122.04	112.60
1	C	152	PHE	CA-CB-CG	5.55	119.35	113.80
1	C	10	ASP	N-CA-CB	5.55	118.65	109.88
1	A	26	LEU	N-CA-C	-5.52	100.19	108.96
1	A	14	ALA	O-C-N	-5.50	117.47	123.52
1	A	47	GLN	N-CA-C	5.49	117.52	109.24
1	B	146	GLU	CA-CB-CG	5.49	125.07	114.10
1	A	59	TYR	CA-C-O	-5.48	115.03	121.44
1	C	91	VAL	CA-CB-CG2	-5.47	101.10	110.40
1	B	154	ILE	CB-CG1-CD1	-5.45	102.35	113.80
1	B	138	ARG	O-C-N	-5.42	116.93	121.27
1	B	15	HIS	CA-CB-CG	-5.41	108.39	113.80
1	B	15	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	C	37	LEU	N-CA-C	-5.40	96.41	107.70
1	C	146	GLU	CA-C-O	5.40	126.85	120.69
1	A	99	SER	CA-CB-OG	5.40	121.89	111.10
1	C	23	GLU	CA-CB-CG	-5.39	103.31	114.10
1	C	64	PHE	CA-CB-CG	5.35	119.15	113.80
1	C	73	HIS	O-C-N	5.34	129.57	122.95
1	A	39	ASN	CB-CG-ND2	5.34	124.41	116.40
1	A	129	GLY	CA-C-O	-5.34	113.56	119.27
1	C	16	VAL	CB-CA-C	5.33	118.71	110.50
1	A	110	GLU	N-CA-C	5.33	122.15	110.80
1	B	113	PRO	CB-CA-C	5.33	117.35	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	ALA	N-CA-C	5.33	122.15	110.80
1	A	13	VAL	N-CA-CB	5.32	119.97	112.52
1	B	111	ALA	CA-C-O	5.30	128.09	120.51
1	B	107	GLU	N-CA-C	5.28	122.05	110.80
1	B	81	SER	O-C-N	5.27	129.73	123.24
1	A	68	GLY	CA-C-O	5.27	129.73	120.57
1	A	82	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	C	89	THR	CA-CB-CG2	5.26	119.44	110.50
1	C	147	SER	N-CA-C	-5.25	99.63	110.80
1	B	25	GLN	N-CA-C	-5.24	100.36	108.42
1	B	56	TYR	CA-CB-CG	5.24	123.33	113.90
1	A	135	GLU	CB-CA-C	-5.21	100.72	109.83
1	C	117	PRO	O-C-N	-5.20	116.50	123.06
1	B	57	LEU	N-CA-C	-5.18	101.32	109.25
1	C	72	THR	CA-CB-CG2	5.18	119.30	110.50
1	C	105	THR	CA-C-N	5.18	126.31	119.84
1	C	105	THR	C-N-CA	5.18	126.31	119.84
1	B	71	SER	O-C-N	5.17	128.96	122.65
1	C	30	ASN	CA-C-N	5.17	131.42	121.54
1	C	30	ASN	C-N-CA	5.17	131.42	121.54
1	B	95	SER	CA-CB-OG	5.17	121.43	111.10
1	B	34	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	C	28	TRP	CB-CG-CD1	-5.16	119.17	126.90
1	A	135	GLU	N-CA-C	5.15	118.14	110.52
1	C	82	ARG	CA-C-O	-5.14	114.86	120.36
1	B	11	LYS	CA-C-N	5.13	126.26	119.84
1	B	11	LYS	C-N-CA	5.13	126.26	119.84
1	A	66	GLY	N-CA-C	-5.12	102.05	110.56
1	A	92	ASN	N-CA-CB	-5.12	102.66	110.65
1	A	109	ALA	N-CA-C	-5.12	98.68	107.23
1	C	109	ALA	O-C-N	5.12	128.06	122.64
1	C	10	ASP	CB-CA-C	-5.11	102.70	110.88
1	A	110	GLU	CA-CB-CG	5.11	124.32	114.10
1	B	30	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	103	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	B	97	ILE	O-C-N	-5.10	118.38	122.97
1	A	39	ASN	CA-CB-CG	5.09	117.69	112.60
1	A	101	CYS	CA-CB-SG	-5.08	102.70	114.40
1	A	78	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	B	7	THR	CA-CB-OG1	-5.07	102.00	109.60
1	A	92	ASN	CA-CB-CG	5.04	117.64	112.60
1	B	37	LEU	N-CA-C	-5.03	100.09	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	B	82	ARG	N-CA-C	-5.00	100.36	108.52
1	B	144	PHE	O-C-N	-5.00	115.07	121.83
1	A	73	HIS	CB-CG-CD2	-5.00	124.70	131.20
1	B	7	THR	CA-CB-CG2	5.00	119.01	110.50
1	B	11	LYS	CA-C-O	-5.00	114.59	119.69

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	THR	Peptide
1	A	7	THR	Peptide
1	B	105	THR	Peptide
1	B	7	THR	Peptide
1	C	11	LYS	Peptide
1	C	146	GLU	Peptide
1	C	7	THR	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1184	0	1181	50	0
1	B	1184	0	1181	67	0
1	C	1184	0	1181	57	0
All	All	3552	0	3543	152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (152) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PRO:HG3	1:C:54:GLY:HA2	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LEU:HA	1:C:148:GLY:HA3	1.60	0.82
1:B:98:LYS:HD2	1:B:116:GLU:HG3	1.65	0.79
1:A:149:GLN:HG3	1:A:150:VAL:H	1.47	0.79
1:C:53:GLU:HG3	1:C:127:GLU:HG3	1.67	0.76
1:B:60:SER:HB2	1:B:80:ILE:HD11	1.69	0.75
1:B:106:PRO:HB2	1:B:111:ALA:HB2	1.69	0.73
1:A:15:HIS:O	1:A:35:ALA:HA	1.88	0.72
1:C:82:ARG:HB2	1:C:93:LEU:HD11	1.71	0.70
1:A:77:THR:HG22	1:A:97:ILE:HG23	1.72	0.70
1:B:77:THR:HG22	1:B:97:ILE:HG23	1.74	0.70
1:C:65:LYS:HD3	1:C:143:LEU:HD12	1.72	0.69
1:C:30:ASN:ND2	1:C:31:ARG:HH22	1.91	0.69
1:A:149:GLN:HG3	1:A:150:VAL:HG12	1.75	0.68
1:A:149:GLN:HG3	1:A:150:VAL:N	2.09	0.67
1:C:47:GLN:OE1	1:C:131:ARG:HB3	1.95	0.67
1:A:146:GLU:O	1:A:149:GLN:HG2	1.97	0.65
1:B:146:GLU:HG3	1:B:149:GLN:HB2	1.79	0.64
1:C:16:VAL:HG12	1:C:152:PHE:HB3	1.79	0.64
1:B:144:PHE:HA	1:B:146:GLU:HB3	1.78	0.63
1:B:103:ARG:HD2	1:B:104:GLU:H	1.62	0.63
1:A:30:ASN:HA	1:A:35:ALA:HB1	1.81	0.63
1:C:19:ASN:OD1	1:C:21:GLN:HB2	1.98	0.62
1:A:87:TYR:HD2	1:A:87:TYR:H	1.47	0.61
1:A:84:ALA:HA	1:A:130:ASP:HB2	1.82	0.60
1:A:62:VAL:HG12	1:A:150:VAL:HG23	1.83	0.59
1:A:69:CYS:O	1:A:105:THR:HA	2.01	0.59
1:B:48:LEU:O	1:B:131:ARG:HA	2.02	0.59
1:B:94:LEU:CA	1:C:148:GLY:HA3	2.33	0.58
1:B:132:LEU:HD13	1:B:154:ILE:HG21	1.86	0.58
1:C:69:CYS:O	1:C:105:THR:HA	2.04	0.58
1:B:65:LYS:HD2	1:B:143:LEU:HD23	1.85	0.57
1:C:14:ALA:HA	1:C:36:LEU:O	2.04	0.57
1:A:67:GLN:HA	1:A:113:PRO:HA	1.85	0.57
1:A:10:ASP:HA	1:A:39:ASN:ND2	2.20	0.57
1:A:9:SER:HB3	1:A:11:LYS:HG2	1.88	0.56
1:C:80:ILE:HA	1:C:133:SER:O	2.05	0.56
1:B:84:ALA:HB3	1:B:88:GLN:HA	1.88	0.56
1:A:155:ILE:HD13	1:C:157:LEU:HD12	1.87	0.56
1:A:106:PRO:HB2	1:A:110:GLU:HA	1.87	0.55
1:A:64:PHE:HA	1:A:141:TYR:O	2.05	0.55
1:A:138:ARG:NH2	1:A:141:TYR:CE1	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SER:CB	1:A:11:LYS:HG2	2.37	0.55
1:B:49:VAL:HA	1:B:130:ASP:O	2.06	0.55
1:B:96:ALA:HB3	1:B:118:ILE:HG21	1.88	0.54
1:B:65:LYS:HD2	1:B:143:LEU:HB2	1.90	0.54
1:C:30:ASN:O	1:C:31:ARG:HB2	2.07	0.54
1:A:13:VAL:HG12	1:A:155:ILE:HB	1.89	0.54
1:C:17:VAL:HG23	1:C:29:LEU:HB3	1.89	0.54
1:C:19:ASN:HD22	1:C:29:LEU:HD23	1.73	0.54
1:A:58:ILE:O	1:A:121:GLY:HA2	2.08	0.54
1:B:60:SER:CB	1:B:80:ILE:HD11	2.38	0.53
1:A:14:ALA:HB2	1:A:41:VAL:HG11	1.89	0.53
1:A:102:GLN:NE2	1:B:114:TRP:HB3	2.24	0.53
1:C:15:HIS:O	1:C:35:ALA:HA	2.08	0.53
1:A:112:LYS:HG3	1:C:102:GLN:HE22	1.75	0.53
1:A:94:LEU:HA	1:B:148:GLY:HA3	1.90	0.52
1:A:57:LEU:HB2	1:A:157:LEU:HD11	1.92	0.52
1:B:94:LEU:HA	1:C:148:GLY:CA	2.36	0.52
1:C:84:ALA:O	1:C:88:GLN:HA	2.10	0.52
1:B:13:VAL:HG23	1:B:155:ILE:HD13	1.90	0.52
1:B:94:LEU:HB3	1:B:120:LEU:HG	1.90	0.52
1:B:144:PHE:C	1:B:146:GLU:H	2.17	0.52
1:B:67:GLN:HA	1:B:113:PRO:HA	1.91	0.52
1:C:79:THR:HG23	1:C:95:SER:HB3	1.90	0.52
1:A:59:TYR:HH	1:C:123:VAL:HB	1.75	0.52
1:A:73:HIS:CE1	1:B:112:LYS:HB3	2.45	0.52
1:B:63:LEU:HD12	1:B:149:GLN:CD	2.35	0.51
1:B:73:HIS:HE1	1:B:102:GLN:HA	1.75	0.51
1:B:103:ARG:HD2	1:B:104:GLU:N	2.25	0.51
1:C:65:LYS:HE2	1:C:143:LEU:HA	1.91	0.51
1:B:80:ILE:HA	1:B:133:SER:O	2.11	0.51
1:C:10:ASP:HA	1:C:39:ASN:ND2	2.26	0.51
1:B:106:PRO:CB	1:B:111:ALA:HB2	2.40	0.51
1:A:103:ARG:HD2	1:B:104:GLU:OE1	2.12	0.50
1:A:136:ILE:HD11	1:A:139:PRO:HA	1.92	0.50
1:C:78:HIS:O	1:C:95:SER:HA	2.11	0.50
1:C:7:THR:HA	1:C:8:PRO:O	2.12	0.50
1:B:43:LEU:HA	1:B:47:GLN:O	2.12	0.50
1:C:98:LYS:HD3	1:C:116:GLU:HG3	1.93	0.49
1:A:59:TYR:OH	1:C:123:VAL:HB	2.12	0.49
1:B:14:ALA:HB2	1:B:41:VAL:HG21	1.93	0.49
1:B:146:GLU:HB2	1:B:149:GLN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:LEU:HD12	1:C:125:GLN:HB2	1.95	0.49
1:B:47:GLN:HG2	1:B:133:SER:HB3	1.94	0.48
1:C:84:ALA:HA	1:C:130:ASP:OD2	2.12	0.48
1:B:79:THR:HG22	1:B:95:SER:HB3	1.96	0.48
1:B:104:GLU:HB3	1:B:106:PRO:HG3	1.95	0.48
1:C:22:ALA:O	1:C:24:GLY:N	2.47	0.48
1:A:92:ASN:HB3	1:B:147:SER:OG	2.13	0.48
1:C:30:ASN:ND2	1:C:31:ARG:NH2	2.61	0.48
1:C:68:GLY:HA2	1:C:106:PRO:HG2	1.96	0.48
1:B:102:GLN:NE2	1:C:114:TRP:HB3	2.28	0.48
1:A:61:GLN:O	1:A:150:VAL:HA	2.14	0.48
1:A:72:THR:OG1	1:B:112:LYS:HE3	2.14	0.47
1:A:84:ALA:HA	1:A:130:ASP:CB	2.43	0.47
1:B:102:GLN:CD	1:C:114:TRP:HB3	2.40	0.47
1:B:125:GLN:OE1	1:C:6:ARG:N	2.48	0.47
1:A:30:ASN:O	1:A:31:ARG:HG2	2.14	0.47
1:B:146:GLU:HB2	1:B:149:GLN:OE1	2.14	0.47
1:B:19:ASN:HB2	1:B:29:LEU:HD13	1.97	0.47
1:B:69:CYS:HA	1:B:70:PRO:HD3	1.72	0.47
1:A:63:LEU:HG	1:A:149:GLN:HB2	1.97	0.47
1:C:17:VAL:HB	1:C:32:ARG:HH11	1.80	0.46
1:C:84:ALA:O	1:C:88:GLN:HG2	2.16	0.46
1:C:94:LEU:HB3	1:C:120:LEU:HD22	1.97	0.46
1:B:73:HIS:CE1	1:B:101:CYS:O	2.69	0.46
1:C:98:LYS:HD2	1:C:118:ILE:HG12	1.97	0.46
1:C:50:VAL:HG21	1:C:126:LEU:HD13	1.97	0.46
1:C:107:GLU:HG3	1:C:108:GLY:H	1.80	0.46
1:B:10:ASP:HA	1:B:39:ASN:OD1	2.16	0.45
1:A:58:ILE:HD11	1:A:126:LEU:HD11	1.98	0.45
1:B:61:GLN:O	1:B:150:VAL:HA	2.17	0.45
1:C:16:VAL:HG22	1:C:29:LEU:O	2.17	0.45
1:B:146:GLU:HB2	1:B:149:GLN:CD	2.42	0.45
1:A:70:PRO:O	1:A:105:THR:HG23	2.17	0.45
1:C:56:TYR:HB2	1:C:126:LEU:HD12	1.98	0.45
1:C:57:LEU:O	1:C:154:ILE:HA	2.17	0.45
1:B:146:GLU:CG	1:B:149:GLN:HB2	2.44	0.45
1:A:92:ASN:HB3	1:B:147:SER:CB	2.46	0.45
1:B:12:PRO:HB3	1:B:51:PRO:HG3	2.00	0.44
1:B:58:ILE:HG23	1:B:154:ILE:HG22	1.99	0.44
1:B:80:ILE:HG13	1:B:120:LEU:HD23	1.99	0.44
1:A:83:ILE:HA	1:A:89:THR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:SER:N	1:B:148:GLY:O	2.51	0.43
1:B:47:GLN:OE1	1:B:131:ARG:HD3	2.18	0.43
1:B:79:THR:HG22	1:B:95:SER:CB	2.48	0.43
1:B:136:ILE:HD13	1:B:142:LEU:HD21	2.00	0.43
1:A:82:ARG:HB2	1:A:93:LEU:HD11	2.01	0.43
1:B:30:ASN:HA	1:B:35:ALA:HB1	2.01	0.43
1:A:8:PRO:HD2	1:C:125:GLN:OE1	2.19	0.43
1:A:12:PRO:HB3	1:A:41:VAL:HG23	2.01	0.42
1:C:32:ARG:NH1	1:C:146:GLU:HB3	2.34	0.42
1:A:30:ASN:CA	1:A:35:ALA:HB1	2.48	0.42
1:C:61:GLN:HA	1:C:118:ILE:O	2.20	0.42
1:A:19:ASN:HA	1:A:29:LEU:HD22	2.00	0.42
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.79	0.42
1:C:110:GLU:OE1	1:C:111:ALA:HB3	2.20	0.42
1:B:20:PRO:HA	1:B:144:PHE:CD2	2.54	0.42
1:A:59:TYR:CZ	1:C:123:VAL:HB	2.55	0.41
1:C:52:SER:O	1:C:128:LYS:HB2	2.20	0.41
1:B:19:ASN:HA	1:B:20:PRO:HD3	1.91	0.41
1:C:82:ARG:NH2	1:C:130:ASP:OD1	2.52	0.41
1:C:32:ARG:O	1:C:34:ASN:N	2.54	0.41
1:A:85:VAL:H	1:A:130:ASP:HB3	1.86	0.41
1:B:15:HIS:O	1:B:35:ALA:HA	2.21	0.41
1:B:83:ILE:HG23	1:B:131:ARG:HB2	2.03	0.41
1:B:146:GLU:HG2	1:B:147:SER:O	2.21	0.41
1:C:83:ILE:CG2	1:C:90:LYS:HG2	2.51	0.41
1:B:59:TYR:HA	1:B:120:LEU:O	2.21	0.41
1:B:97:ILE:O	1:C:115:TYR:HB3	2.22	0.40
1:C:10:ASP:HA	1:C:39:ASN:HD21	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	150/157 (96%)	121 (81%)	19 (13%)	10 (7%)	1	1
1	B	150/157 (96%)	115 (77%)	25 (17%)	10 (7%)	1	1
1	C	150/157 (96%)	111 (74%)	25 (17%)	14 (9%)	0	0
All	All	450/471 (96%)	347 (77%)	69 (15%)	34 (8%)	1	1

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	THR
1	A	100	PRO
1	A	104	GLU
1	A	107	GLU
1	B	84	ALA
1	B	88	GLN
1	B	104	GLU
1	C	23	GLU
1	C	53	GLU
1	C	75	LEU
1	C	106	PRO
1	A	70	PRO
1	A	75	LEU
1	B	24	GLY
1	B	37	LEU
1	B	75	LEU
1	C	26	LEU
1	C	31	ARG
1	C	33	ALA
1	C	52	SER
1	C	108	GLY
1	C	111	ALA
1	A	9	SER
1	A	32	ARG
1	A	110	GLU
1	B	8	PRO
1	B	9	SER
1	B	68	GLY
1	C	51	PRO
1	C	145	ALA
1	A	155	ILE
1	C	39	ASN
1	C	147	SER
1	B	51	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	127/133 (96%)	99 (78%)	28 (22%)	1	2
1	B	127/133 (96%)	98 (77%)	29 (23%)	1	1
1	C	127/133 (96%)	95 (75%)	32 (25%)	0	1
All	All	381/399 (96%)	292 (77%)	89 (23%)	1	1

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	17	VAL
1	A	19	ASN
1	A	29	LEU
1	A	32	ARG
1	A	37	LEU
1	A	39	ASN
1	A	43	LEU
1	A	48	LEU
1	A	52	SER
1	A	55	LEU
1	A	57	LEU
1	A	65	LYS
1	A	70	PRO
1	A	71	SER
1	A	73	HIS
1	A	75	LEU
1	A	76	LEU
1	A	82	ARG
1	A	83	ILE
1	A	85	VAL
1	A	87	TYR
1	A	97	ILE
1	A	105	THR
1	A	120	LEU
1	A	131	ARG

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Mol	Chain	Res	Type
1	A	140	ASP
1	A	154	ILE
1	B	17	VAL
1	B	23	GLU
1	B	29	LEU
1	B	30	ASN
1	B	41	VAL
1	B	43	LEU
1	B	44	ARG
1	B	50	VAL
1	B	53	GLU
1	B	55	LEU
1	B	63	LEU
1	B	65	LYS
1	B	67	GLN
1	B	73	HIS
1	B	76	LEU
1	B	81	SER
1	B	82	ARG
1	B	83	ILE
1	B	85	VAL
1	B	86	SER
1	B	104	GLU
1	B	105	THR
1	B	107	GLU
1	B	110	GLU
1	B	116	GLU
1	B	120	LEU
1	B	126	LEU
1	B	127	GLU
1	B	146	GLU
1	C	12	PRO
1	C	16	VAL
1	C	17	VAL
1	C	23	GLU
1	C	31	ARG
1	C	32	ARG
1	C	36	LEU
1	C	39	ASN
1	C	41	VAL
1	C	42	GLU
1	C	48	LEU

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Mol	Chain	Res	Type
1	C	49	VAL
1	C	51	PRO
1	C	55	LEU
1	C	62	VAL
1	C	67	GLN
1	C	72	THR
1	C	73	HIS
1	C	76	LEU
1	C	82	ARG
1	C	83	ILE
1	C	89	THR
1	C	91	VAL
1	C	99	SER
1	C	101	CYS
1	C	103	ARG
1	C	106	PRO
1	C	112	LYS
1	C	127	GLU
1	C	132	LEU
1	C	133	SER
1	C	140	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	27	GLN
1	A	61	GLN
1	A	102	GLN
1	B	25	GLN
1	B	30	ASN
1	B	73	HIS
1	B	92	ASN
1	B	125	GLN
1	C	30	ASN
1	C	78	HIS
1	C	102	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.